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Fullerenes as carriers of extinction, diffuse interstellar bands and anomalous microwave emission

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Abstract. According to semiempirical models, photoabsorption by fullerenes (single and multishell) could explain the shape, width and peak energy of the most prominent feature of the interstellar absorption, the UV bump at 2175 Å. Other weaker transitions are predicted in the optical and near-infrared providing a potential explanation for diffuse interstellar bands. In particular, we find that several fullerenes could contribute to the well known strong DIB at 4430 Å. Comparing cross sections and available data for this DIB and the UV bump we estimate a density of fullerenes in the diffuse interstellar medium of 0.1–0.2 ppm. These molecules could then be a major reservoir for interstellar carbon. We also study the rotation rates and electric dipole emission of hydrogenated icosahedral fullerenes. We investigate these molecules as potential carriers of the anomalous (dust-correlated) microwave emission recently detected by several cosmic microwave background experiments.

Keywords. Ultraviolet: ISM, (ISM:) dust, extinction, ISM: lines and bands

1. Introduction

In 1985 Kroto and Smalley proposed the existence of a new allotropic form of carbon: the fullerenes (Kroto *et al.* 1985). Their research on samples of vaporized graphite using laser beams, initially aimed to reproduce the chemistry of the atmospheres of carbon enriched giant stars, gave as a result the unexpected discovery of the C_{60} (the 60 carbon atoms fullerene). Subsequent experiments by Kroto and Smalley, and others, showed the existence of carbon aggregates with a larger number of atoms (C_{70}, C_{84}, C_{240}) and established that for an even number of atoms larger than 32, these aggregates were stable. While other molecules have serious difficulties to survive in the interstellar medium, the robustness of C_{60} and of fullerenes in general, strongly support a long survival in the harsh conditions of interstellar space.

Several laboratory experiments (Chhowalla *et al.* 2003) and theoretical studies (Henrard *et al.* 1997, Iglesias-Groth 2004) of the photoabsorption by fullerenes and buckyonions (multishell fullerenes) in the UV suggest that these molecules could be responsible of the most intense feature of interstellar absorption, the so-called ultraviolet bump located at 2175 Å. A significant fraction of interstellar carbon (10–30%) could then reside in fullerene related molecules.

It has been suggested (Webster 1991, 1992, 1993) that fullerenes could also be a carrier of diffuse interstellar bands (DIBs). According to theoretical spectra obtained using semiempirical models (Iglesias-Groth *et al.* 2002, 2003), icosahedric fullerenes and buckyonions (from C_{60} to C_{6000}) present numerous low-intensity bands in the optical and near-infrared, several with wavelengths very similar to well known DIBs. Fullerenes deserve further study as potential carriers of DIBs. For the moment, only two DIBs may have been identified as caused by the cation of C_{60} (Foing & Ehrenfreund 1994).

Finally, hydrogenated fullerenes have been proposed as carriers of the anomalous microwave emission recently detected by several experiments on the Cosmic Microwave Background (Iglesias-Groth 2005, 2006). Under the physical conditions of the interstellar medium these molecules should have spin rates of several to tens of GHz, if as expected they have a small dipole moment, then they would emit electric dipole radiation in a frequency range very similar to the observed for the anomalous microwave emission (Watson *et al.* 2005, Casassus *et al.* 2006).

2. Fullerenes: carriers of interstellar extinction and diffuse bands?

Iglesias-Groth (2004) showed that according to Hückel and Pariser-Parr-Pople models photoabsorption by fullerenes and buckyonions (multishell fullerenes) can explain the shape, width and peak energy of the most prominent feature of the interstellar extinction curve, the UV bump at 2175 Å (Figure 1a). Comparing theoretical cross sections and astronomical data, it was derived a density of fullerenes in the diffuse interstellar medium of 0.1–0.2 parts per million, consistent with findings in meteorites (see e.g., Becker & Bunch 1997).

The same models predict for both fullerenes and buckyonions a large number of weak bands in the optical and near infrared. These bands have strength consistent with those of the strongest DIBs and the number per wavelength interval appears to decrease towards longer wavelengths as it is the case for the DIBs. In Figure 1b the predicted wavelengths for these transitions are compared with the positions of the 16 stronger DIBs known (Herbig 1995). At least 30% of these DIBs coincide (within the precision of the model ∽10 Å) with a theoretical transition of a fullerene or buckyonion, leading to a tentative association of these molecules with the DIBs carriers. Several fullerenes (C_{80}, C_{240}, C_{320}, C_{540}) and buckyonions, present a relatively strong band at energies close to the DIB at 4430 Å. Using the theoretical cross sections and available empirical data on the 4430 Å band we estimate for these fullerenes abundances of 0.1 molecules per million hydrogen atoms in regions of the interstellar medium with excess color index of E(B-V) = 1.0. The same interstellar abundance is obtained from observations of the UV bump and the 4430 Å band. Interestingly, it has been noticed a positive correlation (Désert *et al.* 1995)

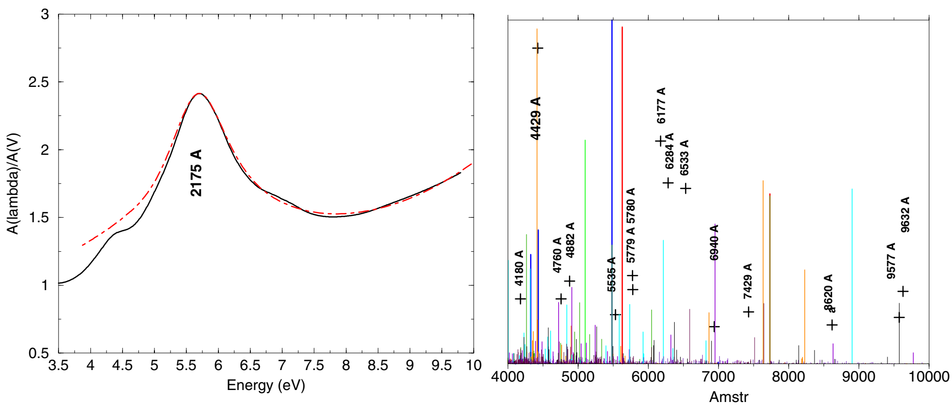

Figure 1. a.- Predicted absorption curves for fullerene and buckyonion mixtures in comparison with observations of the UV 2175 Å bump (5.7 eV) . Extinction curve of the diffuse ISM (dashed red line). Best-fit models to the UV bump obtained for a power-law size distribution $n(R) \propto R^{-m}$ of buckyonions and individual fullerenes ranging from C_{60} to C_{3840}, with index $m = 3.5$ (solid line). b.- Comparison between predicted transitions and the positions of the stronger DIBs known.

between the strength of the UV bump and the strength of various DIBs. The abundances inferred for fullerenes are consistent with estimates for the carbon budget in the ISM.

Hydrides of the fullerene C_{60} have also been investigated as potential DIB carriers (Webster 1993, 1995). No specific identification has been suggested but it should be noted that the conjugated systems of π-electrons are predicted to have transitions in the visible range. The predicted optical and near-infrared transitions of fullerene based molecules may offer a potential explanation for the long-standing problem of the diffuse interstellar bands and other interstellar and circumstellar features.

3. Anomalous Microwave Emission and hydrogenated fullerenes

Recent experiments dedicated to the study of the anisotropy of the cosmic microwave background have found evidence for a new continuum microwave emission in the range 10–100 GHz correlated at high galactic latitudes with thermal emission (DIRBE 100 μm map) from interstellar dust (Kogut *et al.* 1996, Leitch *et al.* 1997, de Oliveira-Costa *et al.* 1999, 2004, Hildebrandt *et al.* 2007). Unambiguous evidence for this new emission mechanism is provided by observations in the Perseus molecular complex (Watson *et al.* 2005) and in the dark cloud LDN 1622 (Casassus *et al.* 2006). An explanation for this dust correlated microwave emission based on electric dipole radiation from small, fast rotating carbon based molecules has been proposed (Draine & Lazarian 1998a). These models appear to reproduce the major features of the so-called anomalous microwave emission (Finkbeiner *et al.* 1999) but do not identify the actual carrier of the emission. Fullerenes and buckyonions fit the basic properties of the carriers proposed in some of the Draine & Lazarian models, particularly the spherical shape and a number of atoms in the range 30-1,000 (required to dominate emission in the 10–100 GHz range). If fullerenes and buckyonions are broadly distributed in the Galaxy and conform a reservoir for interstellar carbon as we have discussed above, they may also play a role as carriers of microwave emission. The reason is that these molecules will be hydrogenated in the interstellar medium. The inhomogeneous distribution of hydrogen atoms in the surface of fullerenes will then cause a net dipole moment because of the polar nature of the C-H bond (0.3 Debyes) and therefore, these molecules are potential carriers of electric dipole emission. As shown by Iglesias-Groth (2006) the same mixture of fullerenes able to explain the UV bump is expected to produce significant microwave emission via electric dipole radiation. The Predicted emissivities calculated using the formalism by Draine & Lazarian (1998a) were compared with very recent measurements of anomalous microwave emission in the Perseus molecular complex (Watson *et al.* 2005) and in the dark cloud LDN 1622 (Casassus *et al.* 2006).

The vibration spectrum of multishell fullerenes may also display bands (Iglesias-Groth & Bretón 2000) in the range 100-500 μm which would correlate with emission at lower frequencies.

4. Conclusions

The cross secction obtained for single fullerenes and buckyonions reproduce the behaviour of the interestellar medium UV extintion curve. A power-law size distribution $n(R) \propto R^{-m}$ with $m = 3.5 \pm 1.0$ for these molecules can explain the position and widths observed for the 2175 Å bump and, partly, the rise in the extintion curve at higher energies. We infer ISM densities of 0.2 and 0.1 ppm for small fullerenes and buckyonions (very similar to the densities measured in meteorites). For a mixture based on single fullerenes and a power-law index of $m = 3.5$ we estimated that $\backsim$ 80 carbon per million hydrogen atoms would be locked in these molecules. If as expected the cosmic carbon abundance is close to the solar atmosphere value, individual fullerenes may lock up 20-25% of the total carbon in the diffuse interstellar space.

Our computations also show that fullerenes and buckyonions present weaker transitions in the optical and near infrared with their number decreasing towards longer wavelengths. These transitions may be responsible for some of the known but unexplained diffuse interstellar bands. It would be very important to obtain high sensitivity, high resolution laboratory spectra of these molecules in the optical and near infrared for a more precise comparison with the very detailed observations of DIBs. Finally, hydrogenated fullerenes and buckyonions are expected to produce rotationally based electric dipole microwave radiation under the conditions of the diffuse interstellar medium. These molecules are potential carriers for the anomalous Galactic microwave emission recently detected by several cosmic microwave experiments.

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Discussion

Cox: The question is about the ionized fullerenes. Could you tell us anything about the possibilities that these are carriers of the diffuse bands?

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Iglesias-Groth: Yes, these molecules could be carriers of DIBs. In fact two transitions of cation of C_{60} were possibly identified in spectra of reddened stars.

Cox: But it's not possible to do any calculations?

Iglesias-Groth: Yes, it is possible to predict their transitions.

Cox: Yes, I mean your calculations on fullerenes, right? So can you do anything on your ionized fullerenes?

van Dishoeck: Have you calculated any ionized fullerenes?

Iglesias-Groth: No, it is not possible using these models. It's an ab-initio calculation.

van Dishoeck: Actually a related question to that is, if you compare your calculated positions of the fullerenes bands, for example, diffuse interstellar bands of 4430 Å, you must have some sort of uncertainty bar on your calculations because there is a relatively simple model of the calculation. Can you estimate what are the uncertainties in your calculations in terms of positions of the bands? For example, for comparison with the data of smaller ones?

Iglesias-Groth: Indeed, these models give approximate wavelengths for the transitions. I think the accuracy is of order 10 Å.

van Dishoeck: What is the uncertainty in the positions of your calculations - you say you have a band of 5 eV or 1 eV or 2 eV, plus or minus. I'm just wondering what's the uncertainties if you're calculating energies.

Iglesias-Groth: In terms of energy they are accurate to the order of 0.01 eV.

van Dishoeck: I suppose you compared and benchmarked them against known observed transitions, but what are the uncertainties for other transitions?

Iglesias-Groth: The available experimental data for C_{60} allows a detailed comparison for this molecule. The models fit the stronger transitions within 0.01 eV.

Unknown: Do you expect the strong correlation between 4430 Å and the UV bump? We looked. It is not there. There does not exist any correlation.

Iglesias-Groth: No correlation in your opinion? But several published papers propose that there is some correlation. I just point out that fullerenes could be responsible of both the UV bump and the 4430 Å DIB.

Getting ready to start on Monday morning.

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